BNL-68154

Submitted to “Microscopy and Microanalysis 2001”, Aug.5-9, Long Beach, CA

PHASE RETRIEVAL FROM TWO DEFOCUSED IMAGES BY THE TRANSPORT-OF-INTENSITY EQUATION FORMALISM WITH FAST FOURIER TRANSFORM

V.V. Volkov, and Y. Zhu
Materials Science Division, Brookhaven National Laboratory, Upton, NY 11973

The problem of phase retrieval from intensity measurements plays an important role in many fields of physical research, e.g. optics, electron and x-ray microscopy, crystallography, diffraction tomography and others. In practice the recorded images contain information only on the intensity distribution $I(x,y) = \Psi * \Psi^* = |A|^2$ of the imaging wave function $\Psi = A * \exp(-i\varphi)$ and the phase information $\varphi(x,y)$ is usually lost. In general, the phase problem can be solved either by special holographic/interferometric methods, or by non-interferometric approaches based on intensity measurements in far Fraunhofer zone or in the Fresnel zone at two adjacent planes orthogonal to the optical axis. The latter approach uses the transport-of-intensity equation (TIE) formalism, introduced originally by Teague [1] and developed later in [2]. Applications of TIE to nonmagnetic materials and magnetic inductance mapping were successfully made in [3,4]. However, this approach still needs further improvement both in mathematics and in practical solutions, since the result is very sensitive to many experimental parameters.

The TIE is derived in paraxial (Fresnel) wave approximation and utilizes a relation of z-gradient for intensity distribution I(x,y) to phase distribution $\varphi(x,y)$ in imaging plane via the 2nd order elliptic differential equation

$$-k\partial_z I = -\nabla_\perp \cdot \left(I \nabla_\perp j\right), \qquad (1) \qquad\qquad \partial_z \iint_\Omega I_z(r_\perp)dr = 0 \qquad (2)$$

with boundary conditions $I(r_\perp)>0$ inside Ω and I=0 on and outside $\delta\Omega=\Gamma$ area. The Eq.(1) can be reduced to Poisson equation via auxiliary equation $\tilde{N} Y = I\tilde{N} j$. It is noted [1,2] that for Eq.(1) the low of energy conservation must hold (Eq.(2)). Recently it was shown [3,4] that serious math problems of Eq.(1) with finite-elements methods can be bypassed by computing of inverse Laplacian $\tilde{N}^{-2}$ via fast Fourier transform (FFT), which gives however only a special solution of Eq.(1). Therefore a problem of unique solution of Eq.(1) in terms of Dirichlet-Neumann boundary conditions remains. Notice that Fourier transform operates only on functions with an infinite support and any real image has to be adopted to FFT by imposing an additional constrains of periodicity $f(x,y) = f(x+2\pi n,y+2\pi m)$ that essentially spoil the recovered j-function at the image boundaries. Hence, the practical way of solving problem is to adopt the Neumann boundary conditions of Eq.(1) to those imposed by the FFT and to use it for determination of unknown coefficients of unique harmonic function $H'(r_\perp)$, with $\tilde{N}^2 H=0$, which contributes to total solution of Eq.(1) as $F = j(FFT) + H'$. This can be realized by two ways. The first one is to apply a zero padding of image using the convolution theorem (a "bad" example is given in Fig1d). The recovered phase in this case suffers from periodicity constrains and is a sensitive function of "zero" mask to the wrap-around problem. The second one, which is a subject of present paper, is to apply the symmetry principles of FFT-solution to problem (1)-(2). By applying the Stoke's theorem we found that Eq.(2) can be reduced to vanished line integral on Γ under condition $\tilde{N} Y = even$, which gives a non-spoiled solution of problem (1) in entire area Ω by constructing the recovered phase as $F = even$. This also dramatically reduces the harmonic function H, ideally, down to one fitting term $D(x^2-y^2)$ The calculation should be performed on $2x2\Omega$ image domain. Some examples of TIE-FFT solution for TEM-phase retrieval of non-magnetic(Fig.1) and magnetic samples (Fig.2) will be discussed. The stability of TIE-solution to noise and to practical image alignment and distortions will be addressed as well.

References:

1. M. E. Teague, J. Opt. Soc. Am. **73**(11), 1434-1441 (1983).
2. T.E. Gureyev, K.A. Nugent, J. Opt.Soc. Am. **A13**(8), 1670-1682 (1996).
3.D. Paganin, K.A. Nugent, Phys. Rev. Letters, **80(**12),2586-2589 (1998).
4. M. De Graef, Y. Zhu, *"Magnetic imaging and its applications to materials"*, Acad. Press, p.295 (2001).
5. Work supported by US DOE, DE-AC02-98CH10886. Stimulating discussions and partial use of the computer codes from M. De Graef are also acknowledged.

BNL-68154

Submitted to "Microscopy and Microanalysis 2001", Aug.5-9, Long Beach, CA

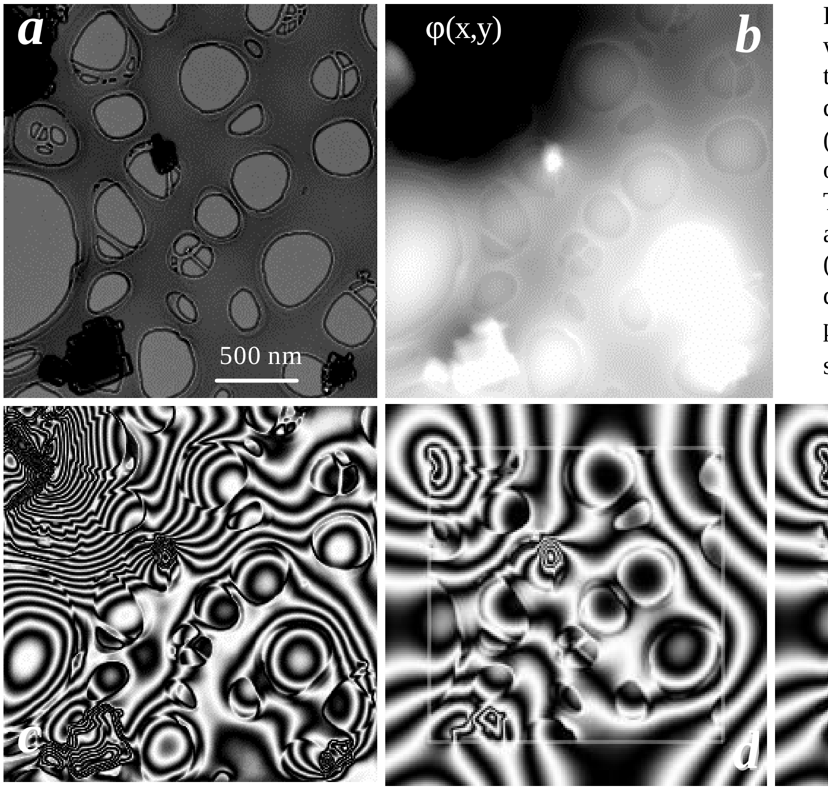

Fig.1 (a) Lacey carbon film with nanoparticles used for the phase recovery from 2 defocused images, (b) reconstructed phase φ obtained by the "even" TIE solution on the domain area $2x2\Omega$, (c) the same phase as (b) displayed by the equal potential contours with 2π spacing, (d) similar solution of TIE on the $1x1\Omega$ area with a mask of 60 pixels (Ω=512x512pixels). Notice, in both cases (c,d) recovered phase reproduces well structure features and thickness variations in (a) , however, in case (d) solution appears to be highly spoiled at the image boundaries.

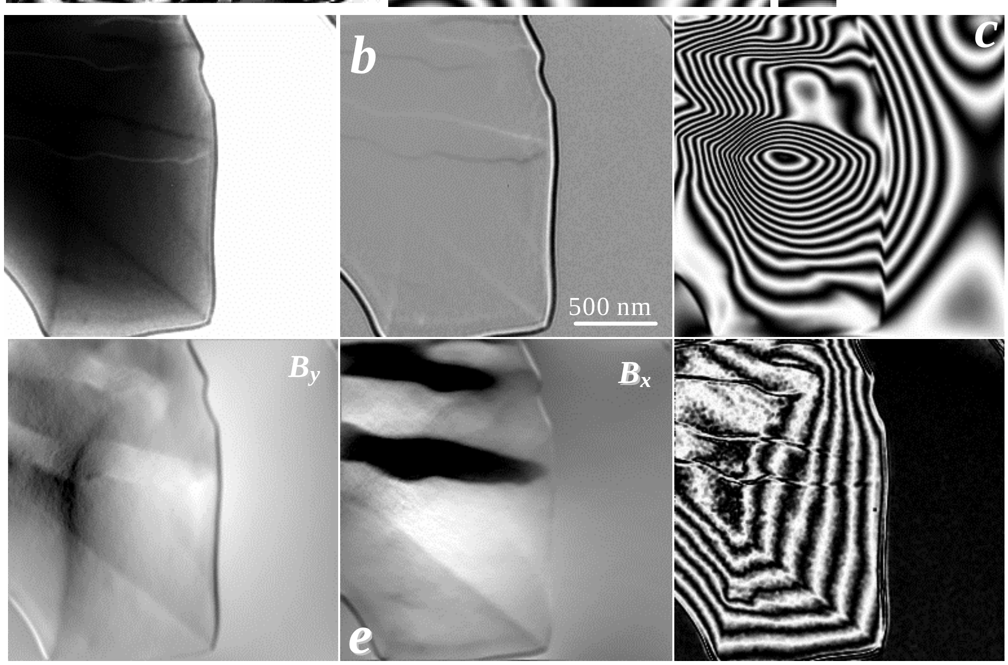

Fig.2 TIE phase retrieval in hard magnet $Nd_2Fe_{14}B$: (a) out-of-focus image showing domain walls, (b) the difference for two out-of-focus images, (c) recovered phase as potential contours with 2π spacing, (d - e) B_y and B_x components of the total magnetization (as simple $\mathrm{grad}_x\varphi$ and $\mathrm{grad}_y\varphi$ respectively), (f) thickness map from the same area with contour spacing of 10 nm. Notice, phase in (c) doesn't follow the thickness profile (f) because of significant contribution of magnetostatic potential in the Nd-Fe-B sample.